

The Anderson Transition in Two-Dimensional Systems with Spin-Orbit Coupling

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We report a numerical investigation of the Anderson transition in two-dimensional systems with spin-orbit coupling. An accurate estimate of the critical exponent ν for the divergence of the localization length in this universality class has to our knowledge not been reported in the literature. Here we analyse the SU(2) model. We find that for this model corrections to scaling due to irrelevant scaling variables may be neglected permitting an accurate estimate of the exponent $\nu = 2.73 \pm 0.02$.

According to the scaling theory of localisation [1], if interactions are neglected, all states are localised in two dimensions (2D). Two exceptions predicted by the scaling theory to this oft recited mantra are the extended states which occur at the center of a Landau level in the quantum Hall effect (QHE) [2], and the Anderson transition which occurs in zero magnetic field if there is a significant spin-orbit interaction [3, 4].

A surprising aspect of the QHE is that the estimate $\nu = 2.35 \pm .03$ [2, 5] for non-interacting electrons of the critical exponent ν , which describes the divergence of the localisation length ξ at the transition, is in close agreement with the measured value. This is despite the fact that interactions are clearly relevant since the dynamical exponent z is predicted to be two for non-interacting electrons while the experimental value is unity.

Critical phenomena are determined by the symmetry of the Hamiltonian and the dimensionality of the system. The important symmetries for the Anderson transition exhibited by non-interacting electrons are time reversal symmetry and spin rotation symmetry. There are three universality classes: orthogonal, unitary and symplectic. Systems with time reversal symmetry but where spin rotation symmetry is broken by the spin-orbit interaction belong to the symplectic class.

In this paper we estimate using numerical simulation and finite size scaling the exponent ν for the Anderson transition in the symplectic universality class in 2D. In contrast to the QHE, where extended states occur only in vanishingly small energy region, the metallic phase extends over a finite energy interval. This system is, therefore, a good candidate for the study of 2D quantum phase transitions. Early work suggested that metallic phase in this model is destroyed when interactions between electrons are taken into account [6, 7], while more recent work suggests that this is not so [8].

Recently, there have been numerous reports of the observation of a zero magnetic field metal-insulator transition in 2D together with measurements of the critical exponents which characterize this transition [9]. Whether or not those experiments indicate the existence of a true

TABLE I: Published estimates of the critical exponent for the 2D symplectic universality class. Q1DLL means finite size scaling for the quasi-one dimensional localization length, ELS energy level statistics and MFSS multifractal finite size scaling. The errors quoted are one standard deviation.

Ref.	model	method	ν
4	Ando model	Q1DLL	2.05 ± 0.08
10	Ando model	Q1DLL	2.75 ± 0.1
11	Evangelou model	Q1DLL	2.5 ± 0.3
12	Ando model	ELS	2.32 ± 0.14
13	network model	Q1DLL	2.51 ± 0.18
14	network model	Q1DLL	2.88 ± 0.15
15	Ando model	MFSS	2.41 ± 0.24

metallic phase at zero temperature remains in dispute. If there is indeed a transition, the physics driving it and whether there is a relation with the transition we study here is not yet clear. However, just as was the case for the QHE, we believe that an accurate estimate for the metal-insulator transition in zero field in non-interacting 2D systems may prove useful.

There has been only very limited success in estimating the critical exponent with field theoretic methods [16, 17]. In Table I we tabulate the estimates of the exponent reported in previous numerical studies [4, 10, 11, 12, 13, 14, 15]. There is considerable variation between these estimates. The estimates reported in [10, 11, 13, 14, 15] seem to be consistent with a true value of the exponent in the range [2.6, 2.9]. However, the estimate of [12] is somewhat below this and that of [4] is in contradiction with the estimates of [10, 14].

We use the transfer matrix method [18, 19] to estimate the localization length λ of electrons on an $L \times L_z$ quasi-1D strip and then extract the critical exponent from a finite size scaling analysis of the dependence of λ on L and disorder. Two important factors limiting the accuracy of the estimate of the exponent obtained in this way are the accuracy of the data for λ and the maximum width

L for which data are available. The standard error in the estimate of λ decreases as $\sqrt{\lambda/L_z}$, while for a fixed L_z the CPU time needed increases as L^3 . At the critical point λ increases linearly with L so that the CPU time needed to estimate λ to a given accuracy increases as L^4 . This means that it is somewhat easier to improve the accuracy of the numerical data than to increase the size of the systems simulated. However, as the accuracy of the raw data improves, corrections to scaling due to irrelevant scaling variables become more important. While such corrections can be taken into account [20], the number of fitting parameters is increased and correspondingly the uncertainty in the estimate of the exponent is increased. It is therefore advantageous to choose a model for which such corrections are negligible even when the raw data are of high accuracy. In this paper we report results for an SU(2) model for which this condition is satisfied.

The Hamiltonian for the SU(2) model describes non-interacting electrons on a 2D square lattice with nearest neighbour hopping

$$H = \sum_{i,\sigma} \epsilon_i c_{i,\sigma}^\dagger c_{i,\sigma} - V \sum_{\langle i,j \rangle, \sigma, \sigma'} R(i,j)_{\sigma\sigma'} c_{i,\sigma}^\dagger c_{j,\sigma'} \quad (1)$$

Here $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) denotes the creation (annihilation) operator of an electron at the site i with spin σ and ϵ_i denotes the random potential at site i . We assume a box distribution with each ϵ_i uniformly and independently distributed on the interval $[-W/2, W/2]$. The width W of the distribution measures the strength of the randomness. The constant V is taken to be the unit of energy, $V = 1$.

The spin-orbit coupling appears in the hopping matrix $R(i,j)$ between each pair of nearest neighbours on the lattice. These matrices belong to the group SU(2) of 2×2 unitary matrices with determinant one. The hopping matrices are parameterised as follows

$$R(i,j) = \begin{pmatrix} e^{i\alpha_{i,j}} \cos \beta_{i,j} & e^{i\gamma_{i,j}} \sin \beta_{i,j} \\ -e^{-i\gamma_{i,j}} \sin \beta_{i,j} & e^{-i\alpha_{i,j}} \cos \beta_{i,j} \end{pmatrix} \quad (2)$$

This matrix describes a rotation of the electron spin in three dimensional space. (The Euler angles of this rotation are related to, but not equal to, the angles α , β and γ .) In the SU(2) model the distribution of these angles is chosen so that the $R(i,j)$ are uniformly distributed with respect to the group invariant measure (Haar measure) on SU(2). This corresponds to α and γ uniformly distributed in the range $[0, 2\pi)$, and β distributed according to the probability density,

$$P(\beta)d\beta = \begin{cases} \sin(2\beta)d\beta & 0 \leq \beta \leq \frac{\pi}{2} \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

Hopping matrices on different bonds of the lattice are statistically independent. Periodic boundary conditions

are imposed in the transverse direction. The necessary calculations are carried out using quaternion arithmetic [4] which halves the required number of multiplications compared with an implementation using complex arithmetic.

Some of the physics of the SU(2) model can be understood by comparing it with the Ando model which has been adopted in [4, 10, 12, 15]. In the Ando model as the electron propagates through the material its spin precesses at a rate and about an axis which depend on the electrons wave number. When scattered by the random potential, the rate and the axis about which the electron's spin rotates changes. This leads to a diffusive motion of the spin with an associated spin relaxation length. Quantum interference between time reversed electron trajectories longer than this length produces the weak anti-localization effect [21]. Motivated by the conjecture that the spin relaxation length might be an important irrelevant length scale, we adopted the SU(2) model where the uniform distribution of the hopping matrices on SU(2) ensures that the spin relaxation length is the shortest possible. Doing so we do indeed find that corrections due to irrelevant scaling variables can be neglected.

To determine the critical exponent ν , critical disorder W_c and other critical properties of the transition we fit dependence of $\Lambda = \lambda/L$ on the system size L and the disorder W , or when $W = 0$ on the Fermi energy E_F , to a one parameter scaling law of the form

$$\ln \Lambda = F(\psi). \quad (4)$$

Here ψ is the relevant scaling variable. We expand the scaling function as a power series

$$F(x) = \ln \Lambda_c + x + a_2 x^2 + \dots + a_{n_0} x^{n_0} \quad (5)$$

terminating the expansions at order n_0 . To allow for non-linearity of the scaling variable, the scaling variable is approximated by an expansion in terms of the dimensionless disorder $w = (W_c - W)/W_c$, where W_c is the critical disorder separating the insulating and metallic phases. (If $W = 0$ we set $w = (E_F - E_c)/E_c$.) The growth of the relevant scaling variable with system size is described by the critical exponent ν

$$\psi = L^{1/\nu} (\psi_1 w + \psi_2 w^2 + \dots + \psi_{n_\psi} w^{n_\psi}), \quad (6)$$

where we terminate the expansion at order n_ψ . This same exponent describes the divergence of the localization (correlation) length

$$\xi = \xi_\pm |\psi_1 w + \psi_2 w^2 + \dots + \psi_{n_\psi} w^{n_\psi}|^{-\nu}. \quad (7)$$

where we terminate the expansion at order n_ψ . The absolute scales ξ_\pm of the localization length on either side of the transition are not determined in this analysis, so we set them both to unity for simplicity. The linear coefficient in the expansions of F is set to unity, as shown,

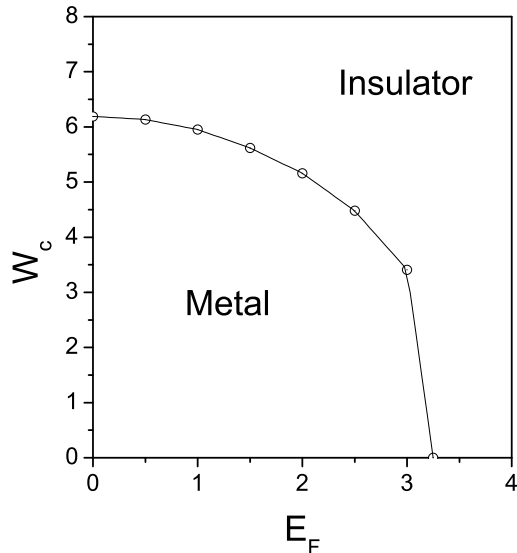


FIG. 1: The phase diagram for the SU(2) model.

to eliminate some redundancy in the definition of the fitting parameters. The total number of parameters is $N_p = n_0 + n_\psi + 2$.

The best fit is determined by minimizing the χ^2 statistic. The quality of the fit is assessed with the goodness of fit probability Q . Confidence intervals for the fitted parameters are estimated using a Monte Carlo method [22]. This involves using the model and the best estimates of the fitting parameters to generate an ideal data set. From this data set a large ensemble of synthetic data sets is generated by adding random errors, with a variance equal to that of the error of the corresponding data point, to the ideal data set. Fitting of the ensemble of synthetic data sets produces a distribution for the critical parameters from which confidence intervals and the goodness of fit are estimated. This procedure is standard and systematic but does not take into account any unknown systematic effects that might only be discernible for very much larger systems. Of course, this caveat applies to almost any numerical estimate of a critical exponent.

Before turning to the estimate of the critical exponent we sketch the phase diagram in Figure 1. The figure is based on data for systems with sizes ranging from $L = 8$ to $L = 32$ for a number of Fermi energies between $E_F = 0$ and $E_F = 3$ for which the critical disorder W_c was estimated, and on data for $W = 0$ for which the critical energy E_c was estimated. In the absence of a random potential i.e. when $W = 0$, the Hamiltonian may have chiral symmetry and, in addition to the transition at finite E_c , a critical state may also be present at the band center [23]. Whether this possibility is realised depends on the boundary conditions and whether the number of

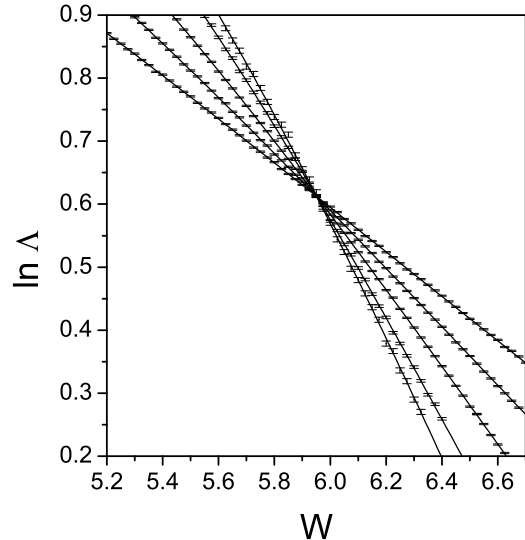


FIG. 2: The numerical data for the SU(2) model and the best fit. Data for $L = 8, 16, 32, 64$ and 96 are shown.

TABLE II: The details of various fits to the numerical data for the SU(2) model. The fit is to $N_d = 230$ data points in the range $5.2 \leq W \leq 6.7$ and $0.2 \leq \ln \Lambda \leq 0.9$.

n_0	n_ψ	N_p	Q	W_c	$\ln \Lambda_c$	ν
2	2	6	0.2	$5.952 \pm .002$	$0.612 \pm .001$	$2.74 \pm .01$
3	2	7	0.4	$5.952 \pm .002$	$0.612 \pm .001$	$2.73 \pm .02$
4	2	8	0.3	$5.952 \pm .002$	$0.612 \pm .001$	$2.73 \pm .02$
3	3	8	0.3	$5.952 \pm .002$	$0.612 \pm .001$	$2.74 \pm .03$
4	3	9	0.3	$5.952 \pm .002$	$0.612 \pm .001$	$2.73 \pm .03$

sites is even or odd. Since chiral symmetry is broken by a random potential it does not affect our estimation of ν below.

To estimate the critical exponent accurately more extensive simulations were carried out for a single energy $E_F = 1$. The numerical data are presented in Figures 2 and 3. Data with an accuracy of 0.1% are available for

TABLE III: The variation of the estimates of the critical parameters for the SU(2) model as data for smaller systems sizes are progressively excluded from consideration. Here $n_0 = 3$ and $n_\psi = 2$.

	N_d	Q	W_c	$\ln \Lambda_c$	ν
$8 \leq L \leq 96$	230	0.4	$5.952 \pm .002$	$0.612 \pm .001$	$2.73 \pm .02$
$16 \leq L \leq 96$	169	0.6	$5.953 \pm .003$	$0.611 \pm .002$	$2.75 \pm .02$
$32 \leq L \leq 96$	113	0.5	$5.954 \pm .005$	$0.611 \pm .003$	$2.71 \pm .04$
$64 \leq L \leq 96$	64	0.8	$5.96 \pm .02$	$0.60 \pm .02$	$2.8 \pm .2$

TABLE IV: The variation of the estimates of the critical parameters for the SU(2) model as the range of disorder under consideration is progressively narrowed.

W	N_d	n_0	n_ψ	Q	W_c	$\ln \Lambda_c$	ν
[5.2, 6.7]	230	3	2	0.4	$5.952 \pm .002$	$0.612 \pm .001$	$2.73 \pm .02$
[5.5, 6.4]	175	2	2	0.7	$5.953 \pm .003$	$0.612 \pm .001$	$2.75 \pm .02$
[5.8, 6.1]	65	1	1	0.5	$5.950 \pm .002$	$0.613 \pm .002$	$2.72 \pm .07$

system sizes $L = 8, 16$ and 32 , with accuracy 0.2% for $L = 64$, and 0.4% for $L = 96$. This required L_z of the order of 10^7 to 10^8 depending on the size, the disorder and the accuracy. When fitting the data the intervals of W and $\ln \Lambda$ to consider must be decided. The exact choice is not particularly important provided all data are in the critical regime. A larger interval of $\ln \Lambda$ requires a higher order of expansion in Eq. 5, while a larger interval of W requires a higher order expansion in Eq. 6. The results of the finite size analysis are presented in Tables II, III and IV. A number of fits of the numerical data are possible but, as can be seen by referring to Table II, all yield consistent results. The estimates of the critical parameters are also stable against restriction of the system sizes under consideration, see Table III, and against a narrowing of the range of disorder, see Table IV. The lines shown in Figure 2 and 3 correspond to a fit with $n_0 = 3$ and $n_\psi = 2$. To demonstrate single parameter scaling graphically we re-plot the data as a function of L/ξ in Figure 3; metallic and insulating branches are clearly visible. These are described by related scaling functions F_+ and F_- where

$$F_{\pm}(x) = \ln \Lambda_c \pm x^{1/\nu} + a_2 x^{2/\nu} + \dots + (\pm 1)^{n_0} a_{n_0} x^{n_0/\nu} \quad (8)$$

In summary, we have studied the Anderson transition in the 2D symplectic universality class and estimated the critical exponent ν . We find $\nu = 2.73 \pm .02$, where the error is a 95% confidence interval. Our result is consistent with the estimates reported in [10, 11, 13, 14, 15] but not with those of [4, 12]. Analyses based on energy level statistics, such as [12], also seem to have a tendency to produce estimates which are lower than those of the transfer matrix method for the 3D orthogonal universality class [24]. On the other hand, in our opinion, the error bar for the exponent claimed in [4] is too optimistic.

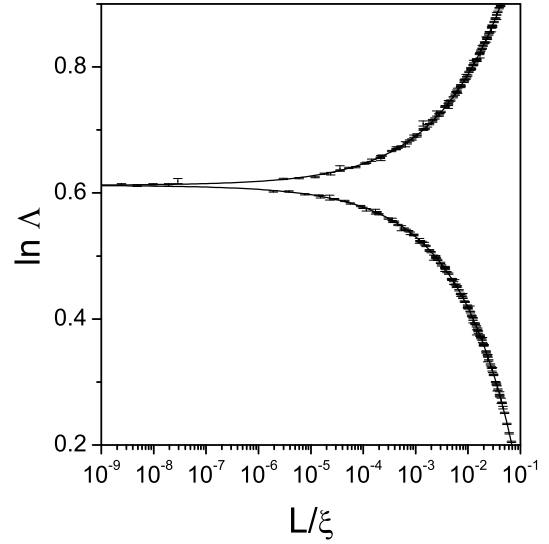


FIG. 3: When plotted versus L/ξ the data divide naturally into an upper metallic branch $F_+(L/\xi)$ and a lower insulating branch $F_-(L/\xi)$.

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